# jems GUI

Dr. Pierre Stadelmann  
Chemin Rouge 15  
CH-1805 Jongny

August 2, 2022

## Contents

1 Introduction  
1.1 Starting jems ......................................... 13

2 Main frame  
2.1 Console .................................................. 14  
2.2 Menus .................................................... 16  
2.3 Tool buttons ............................................. 16
2.4 Popup menus ............................................ 17

3 Importing crystal structures from CIF files  

4 Crystal builder  
4.1 Tool buttons ............................................. 22  
4.2 Tabs ....................................................... 23  
4.3 Atoms table’s tool buttons ............................... 24  
4.4 Crystal builder $\rightarrow$ **Atom** dialogue .......... 25  
4.5 Crystal builder $\rightarrow$ **Space-group** dialogue .. 27  
4.6 Regular **Point** System code dialogue .............. 28

53 Perspective  
53.1 Popup menu ............................................. 172
53.2 Tool buttons ............................................. 172  
53.3 Tabs ..................................................... 173

6 SAED patterns ........................................... 37
27.1 Tool buttons .................................................. 147

28 Rings pattern ........................................ 148
  28.1 Tool buttons .............................................. 148

29 Atomic Form Factor ................................ 150
  29.1 Tool buttons .............................................. 151
  29.2 Popup menu .............................................. 151

30 Structure factors dialogue ....................... 156
  30.1 Tool buttons .............................................. 156

31 Miscellany menu ........................................ 158
  31.1 Miscellany menu items ............................... 158
    31.1.1 Load image .......................................... 159
    31.1.2 Load super-cell ..................................... 160
    31.1.3 Make void ........................................... 161
    31.1.4 To core-shell ....................................... 162
    31.1.5 To particle .......................................... 164
    31.1.6 To precipitate ....................................... 165
    31.1.7 To slices ............................................ 167
    31.1.8 To triclinic ......................................... 168

32 Thickness ................................................ 169
  32.1 Tool buttons .............................................. 169

33 Perspective .............................................. 171
  33.1 Popup menu .............................................. 172
  33.2 Tool buttons .............................................. 172
  33.3 Tabs ..................................................... 173

34 Indexing SAED patterns .............................. 177
  34.1 Tool buttons .............................................. 177
  34.2 Tabs ...................................................... 179
  34.3 Example ................................................ 181

35 ADF imager .............................................. 182
  35.1 Tool buttons .............................................. 183
  35.2 Tabs ...................................................... 184

36 Probe imager ............................................. 192
  36.1 Tool buttons .............................................. 192
## List of Figures

1. jems main window, MacOSX version. .................................. 14  
2. (a) Console and (b) debug panel. ................................... 15  
3. Menus of the menu bar. ................................................. 16  
4. Popup menus attached to the main window left (a) and right (b) panels. ......................................................... 18  
5. Mathematica 3-D view (a) and projected potential (b) of AuCu$_3$. Image popup menu (c) and coloured image (d). ............. 19  
6. CIF data set selector dialogue. ........................................ 20  
7. Hexagonal Bismuth ferrate in [001] and [100] projections. ....... 21  
8. Space-group dialogue to confirm R 3 c space-group settings. ....... 21  
9. Crystal builder frame. ................................................... 22  
10. ZnTe diffraction patterns. ............................................ 23  
11. Crystal builder $\rightarrow$ Atoms tabs. .............................. 23  
12. Crystal builder $\rightarrow$ Cut, Drawing, Duplicate & View tabs. ................................................................. 24  
13. Crystal builder $\rightarrow$ System tabs. ............................... 25  
14. Crystal builder allows to build large super-cells. .................... 25  
15. Atom dialogue. .......................................................... 26  
16. Tables of the Atomic Form Factors. ................................ 27  
17. Space-group dialogue (orthorhombic unit cell). .................... 28  
18. RPS code dialogue for entering the regular point system code. 29  
19. RPS code editor. ...................................................... 30  
20. ZnTe perspective view. ................................................ 171  
21. 3-D view popup menu. ............................................... 172  
22. 3-D view of ZnTe models. .......................................... 173  
23. Controls of 3D-perspective. ........................................ 174  
24. Atoms and Display Tabs. .............................................. 175  
25. Modified 3-D views. .................................................. 176  
26. SAED patterns frame. ................................................. 37  
27. Experimental SAED with a magnified area (yellow square). ....... 39  
28. Table of the plotted reflections. .................................... 40  
29. First 6 tabs of SAED plotting controls. ............................. 41  
30. Last 3 tabs of SAED plotting controls. ............................. 42  
31. ................................................................. 43  
32. SAED images .......................................................... 44  
33. Typical SAED drawing sliders. ...................................... 45  
34. SAED 2-D image and 3-D view. ..................................... 46  
35. Dynamical SAED calculation controls. .............................. 47  
36. Plot of the intensity/phase of reflections as a function of crystal thickness. ..................................................... 47
Mathematica plots of the \((0, 1, 0)\) reflection intensity and phase (modulo \(2\pi\)).

SAED precession settings, camera length 2000 [\(nm\)], deviation 0.1 [\(nm^{-1}\)], tilt 3.0 [\(deg\)].

SAED precession.

Bloch-wave calculations frame.

Reflections table.

Tabs of the different Bloch-wave calculations.

\(AuCu_3\) \((8 \times 8)\) HREM images map with decreasing defocus (horizontally) and increasing thickness (vertically).

Controls the illumination, defocus, specimen thickness values, number of \textit{strong} reflections and introduces Bethe approximation.

Controls to introduce the camera MTF in the HRTEM simulations.

Low magnification.

High magnification.

Effect of 3-fold astigmatism on HRTEM images.

Tool boxes of \textit{Diffraction} (a), \textit{Map} (b) and \textit{Plot} (c) contexts.

\(ZnTe\) \([1, 1, 0]\) CBED pattern calculation.

CBED controls tabs.

CBED controls tabs.

CBED patterns.

Tilted CBED patterns.

LACBED patterns, \((001)\) reflection (bright field).

Multislice frame.

Tabs of multislice calculations frame.

Tabs of multislice calculations frame (continued).

\textit{HREM} \(\rightarrow\) \textit{Multislice} tabs.

HAADF image calculation.

HRTEM imager frame (activated with the largest crystal thickness).

HRTEM imager, right tabs.

Aberrations, CLC and Coherence tabs.

Dark field, Defocus and Defocus series tabs.

Drift/Noise, Holography and Imaging tabs.

Objective aperture and beam stop & phase shift \([deg]\) tabs.

HRTEM imager, objective aperture settings.

\textit{Zernike phase contrast} with out of axis objective aperture and a beam stop that phase shifts the transmitted beam and \{100\} reflections.
HRTEM imager, objective aperture settings. ........................................... 85
HRSTEM imager. ....................................................................................... 86
HRSTEM imager controls. ........................................................................ 87
HRSTEM imager (HAADF image, Probe & Intensity tabs ... 88
Introducing 3-fold astigmatism. ................................................................. 88
Effect of source size change. ................................................................. 89
Imaging x & y image-tiling. ................................................................. 90
Camera MTF frame. ................................................................................ 91
Crystal MTF → tabs. ........................................................................... 92
Data only load dialogue and fitted parameters table. ............................ 93
1024 × 1024 Gatan CCD camera noise, diffractogram, profiles. ............... 93
Mathematica normalized NTF plots. ..................................................... 94
Apertures dialogue. .............................................................................. 95
Objective aperture dialogue tabs. .......................................................... 96
HRTEM images with different objective aperture settings. ....... 96
Effect of the optical axis shift (not to be confused with a crystal tilt). . 97
Use the arrows tool buttons to decrease/increase the number of plotted zone axis. [uvw] zone indices can be entered directly (keyboard return key to confirm). ................................................................. 99
Use the arrows tool buttons to move the Center of the Laue Circle 
(CLIC). ................................................................................................. 100
The deviation slider defines the maximum distance of a reflection 
to the Ewald sphere. ........................................................................ 101
The foil normale sets the angle of the normale to the entrance surface 
of the tilted foil. ................................................................................ 102
The arrow tool buttons increase/decrease the number of Laue zones. 102
The Keeper dialogue keeps most jems parameters. ............................. 103
Wave-front aberrations defined to order 8. ............................................ 105
ADF imager, Diffraction and Imaging tabs. .......................................... 106
Kikuchi and SAED patterns indexing. .................................................. 106
Parameters related to Bloch-wave and multislice calculations. ............ 107
Microscope, precession and vibration parameters. ............................... 107
Wave-front aberration and Contrast Transfer Function. ................. 108
Wave-front aberrations. ..................................................................... 109
Contrast Transfer Function (CTF). ...................................................... 110
Diffractogram and Optical Transfer Function. ................................... 111
Probe shape and Ronchigram. ............................................................. 111
Aberrations and coherence settings. ..................................................... 112
Table of atomic form factors.

Fe atomic form factor (WKc) as a function of $\frac{\sin \theta}{\lambda} = 0$.

Comparison of the Electron Scattering Amplitudes of the different references at $\frac{\sin \theta}{\lambda} = 0$.

AFF sources.

Comparison of the Electron Scattering Amplitudes of the different references at selected $\frac{\sin \theta}{\lambda}$ values.

Scattering angle [mRad] as a function of s [nm$^{-1}$] for selected accelerating voltages [kV]. Note the factor 2 for the conversion nm$^{-1}$ to mRad.

Table of ZnTe structure factors.

Table of non-equivalent ZnTe structure factors and their multiplicity.

Miscellany menu Load image frame.

Miscellany menu Load super-cell frame.

Miscellany menu Make void frame.

Miscellany menu To core-shell frame.

Miscellany menu To core-shell 3D-views. The model is embedded in a box of dimensions large enough to avoid "wrap around" artefacts during the multislice image calculation.

Miscellany menu To particle frame.

Miscellany menu To precipitate frame.

Miscellany menu To precipitate 3D-views. The model is embedded in a box of dimensions large enough to avoid "wrap around" artefacts during the multislice image calculation.

Miscellany menu To slices frame.

Table of slices and 3D-view of a single slice or the stack of slices.

Miscellany menu To triclinic frame.

To triclinic simple model and duplicated void model 3D-view.

Thickness measurement.

Table of non-equivalent ZnTe structure factors and their multiplicity.

ZnTe perspective view.

3-D view popup menu.

3-D view of ZnTe models.

Controls of 3D-perspective.

Atoms and Display Tabs.

Modified 3-D views.

Indexing SAED patterns.

Controls and tabs of SAED patterns indexing.

Controls and tabs of SAED patterns indexing.

Indexing SAED to identify and list the diffraction spots.
The ADF detector dialogue allows to set the size and position of the Bright and Dark field detectors as well as the Sector detector.

ADF imager controls tabs.

Bright field, Dark field, Sector and HAADF image tabs.

Projection, Projected potential, absorption potential, Fresnel propagator image tabs.

Phase object, Power spectrum, Bright field detector, Dark field detector image tabs.

Dark field detector and Wave-function image tabs.

Probe dialogue and Aberrated probe shape 2-D and 3-D (3-fold astigmatism).

Probe imager dialogue.

Probe aberrations.

Coherence, Contrast, Drift&Noise, Microscope settings.

Probe position and probe shape.

Lateral probe view and probe profile (obtained using the attached popup menu).
List of Tables
1 Introduction

This document describes jems Graphical User Interface (GUI). The GUI shows little variations depending on the operating system, i.e. MacOSX, Windows or Linux. The GUI of the MacOSX version is introduced in this document.

1.1 Starting jems

On MacOSX, jems is an ordinary application. On Windows or Linux jems is started using a command file (either .bat or .sh). At startup the About window is briefly visible and shows the jems version. Loading the jems application takes several seconds since many classes stored as java classes are translated (compiled) into machine code.

2 Main frame

jems main window (Fig. 1) displays 2 panels, the left panel lists the atoms of the structure displayed on the right panel. Atoms of the unit cell generated by the translations of the Bravais lattice are not listed. Popup menus are attached to each panel (see paragraph 2.4).
2.1 Console

At startup a scrollable console frame opens that displays information about the user, host and license (Fig. 2a). The console will display more information depending of the debugging options selected in the Parameters → Preferences dialogue → Debug tab (Fig. 2b)\(^1\). Its content can be copied/paste as text file in any text editing program. The console can be closed if convenient.

For example, with the CIF debug option selected, loading a structure provided as a .cif file the console window will display information about the content of the file (not shown here). This information may help detect wrong CIF content.

---

\(^1\)Its whole content can be selected and copy/paste into any text editing program.
(a) Console frame (MacOSX version).

(b) Preferences dialogue, debug panel.

Figure 2: (a) Console and (b) debug panel.
2.2 Menus

The menu bar organises the different menus as usual (Fig. 3). jems student version presents a different menu bar: menu Miscellany is missing and several other menus do not offer some menu items found in the licensed version.

(a) File.  (b) Crystal.  (c) Drawing.  (d) Imaging.  (e) Indexing.  (f) Measuring.  (g) Parameters.  (h) Window.  (i) Miscellany.  (j) Help.

Figure 3: Menus of the menu bar.

2.3 Tool buttons

Most of the tool buttons duplicate a particular menu item in order to access it faster. Only (Transfer to clipboard), that put a copy of the main window (or any window displaying it) in the clipboard, does not duplicate a menu item.

A tip text is attached to every tool button and describes its function. The tip text is shown when the mouse or pointer is moved on the tool button. For example the tip text of is simply "Transfer to clipboard".

The tool buttons of the main window allow to:

- : load a crystal structure in .txt format.
- : print the atoms table.
• _ANALYSIS: save the atoms table in .txt format.
• _ANALYSIS: transfer a frame or dialogue to the clipboard.
• _BUILD: Build a crystal structure (Fig. 9).
• _ATOM: open the Atom dialogue (Fig. 15).
• _REG: open the Regular Point System (RPS) code dialogue (Fig. 18).
• _SPACE: open the Space-group dialogue (Fig. 17).
• _ANT: tabulate the Atomic Form Factors (AFF) (Fig. 16).
• _SAE: plot Selected Area Electron Diffraction patterns (SAED) (Fig. 26).
• _PERS: show Perspective views of crystal structures (Fig. 166).
• _STER: plot [u,v,w] and (h,k,l) Stereographic projections (Fig. 117).
• _CT: define the Contrast Transfer Function (CTF) and Optical Transfer Function (OTF) (Fig. 101).
• _POW: plot Powder pattern (line position) for electron, neutron and X-Ray (Fig. 120).
• _MIC: open the Microscope dialogue (Fig. 112).
• _APET: open the Apertures dialogue (Fig. 83).
• _WAV: show the Wave-front aberrations dialogue (Fig. 100).
•  SPEC: show the Specimen dialogue (Fig. 88a).
•  CRYST: open the Crystallographic calculator (Fig. 114).
•  KEEPER: open the Keeper dialogue (Fig. 94).
•  HELP: display a Help file.

The Help tool button (HELP) is available on each dialogue and frame.

2.4 Popup menus

A double mouse click (or using a touchscreen a double finger or pointer touch) on the left or right panel of the main window displays a popup menu (Fig. 4). Attach

2Depending on the dialogue or frame context some of the tool buttons may have a different functionality (described by the tip text)
to a list the popup menu allows to save, print or transfer the list (as an image) to the clipboard. Attached to other GUI elements each popup menu item allows to modify the content of the panel or to create new images, etc.

For example the popup menu item Export to Mathematica creates a simple Mathematica notebook showing the AuCu$_3$ crystal structure (Fig. 5a). By default the notebook is saved in the default folder, i.e. where the displayed structure is loaded from. As a second example Show projected potential generates the image of the projected potential of AuCu$_3$ (Fig. 5b). Note that the toolbar of the image frame contains tools to process the image and that a popup menu is attached to the image (Fig. 5c) allowing to modify the image (Fig. 5d).

This short document will not described all the simulation and plotting options offered by jems. Only a couple of simulation/plotting frames will be described. The user is urged to refer to these frames in order to figure out how the not described frames perform.

---

3It is always a good idea to create a default folder containing the crystal structure.
(a) $AuCu_3$ crystal structure displayed using Mathematica (arrows: red x, green y, blue z).

(b) $AuCu_3$ projected potential in [0,0,1] direction.

(c) Popup menu attached to the projected potential image.

(d) Coloured projected potential (temperature map).

Figure 5: Mathematica 3-D view (a) and projected potential (b) of $AuCu_3$. Image popup menu (c) and coloured image (d).
3 Importing crystal structures from CIF files

Menu item **File → Import CIF** imports crystal structures defined as .cif files provided by databases like the *Crystallography Open Database*, *American Mineralogist Crystal Structure Database* or *Inorganic Crystal Structure Database*.

Fig. 6 shows the dialogue for selecting a crystal structure in a .cif file containing 50 related Bismuth ferrates structures.

![CIF data set selector dialogue.](image)

The selected structure can be observed in [001], [100] or [010] projections. The select button selects the structure and closes the dialogue (Fig. 7).

It is then necessary to confirm the CIF structure space-group settings since non-conventional settings are not uncommon in crystallographic data bases (Fig. 8).
(a) [001] projection.  
(b) [100] projection. 

Figure 7: Hexagonal Bismuth ferrate in [001] and [100] projections.

Figure 8: Space-group dialogue to confirm $R\ 3\ c$ space-group settings.
4 Crystal builder

The Crystal Builder (CB) is started using menu item Crystal → Builder (Fig. ??) (or main window’s tool button ). It opens with the crystal structure displayed in the main window. The CB uses java3D and is only available when an opengl driver is installed on the computer. The CB allows to build and save crystal structures not distributed with jems.

![Crystal builder frame](image)

Figure 9: Crystal builder frame.

4.1 Tool buttons

The crystal builder tool buttons allow to:

- : print the crystal structure drawing.
- : save the crystal structure drawing.
- : transfer the frame to the clipboard.
- : open the space-group dialogue (Fig. 17).
• : plot an ab-initio electron diffraction powder pattern (Fig. 10a).
• : plot SAED diffraction patterns (Fig. 10b).
• : duplicate the unit cell \( n_x \times n_y \times n_z \) times (Fig. 14c).
• : display a help file.

(a) Ab-initio powder pattern of ZnTe a 8x8x8 unit cells crystallite.
(b) SAED pattern (single scattering).

Figure 10: ZnTe diffraction patterns.

4.2 Tabs

(a) Atoms table.  
(b) Bonds selection.  
(c) Atoms and bonds resolution.  
(d) Atom colour and size selection.

Figure 11: Crystal builder → Atoms tabs.
4.3 Atoms table’s tool buttons

The tool buttons of the atom table allow to:

- ➕: define a new atom position.
- ➖: delete the selected atom.
- 🗑: erase all the atoms.
- 📊: modify the selected atom.
- 📜: save the atoms table as a .txt file.

The ➕ and ➖ open the **Atom** dialogue (Fig. 15), see section 4.4.

When an atom of the 3-D drawing is selected (white sphere) it is identified in the **Atom** text field. All the equivalent atoms of the 3-D drawing are identified when an entry of the table is selected (white spheres).

![Figure 12: Crystal builder → Cut, Drawing, Duplicate & View tabs.](image)

(a) (hkl) cut plane selection.
(b) Drawing options and \([uvw]\) viewing direction.
(c) Unit cell duplicating options.
(d) 3-D viewing selection.

---

4The Wyckoff symbol and AFF source are only saved when the builder frame is closing.
4.4 Crystal builder $\rightarrow$ Atom dialogue

Figs 15a and 15b show the atom dialogue tabs. It is necessary to first select the atom symbol (Atom tab) and then, using the controls of the Coordinates tab, to set the fractional atom coordinates (with the help of the Wyckoff position symbol), Debye-Waller temperature factor, occupancy and absorption. When either the Weickenmaier-Kohl WK or WKc. Atomic Form Factor (AFF) source is selected the absorption should be set to 0.0 since it is always calculated. The dialogue emits a message when the atom site is already partially or fully occupied. In such a case push the Reset button. The Add and Done buttons updates
the atoms table and closes the dialogue respectively.

(a) Atom selection.  
(b) Fractional coordinates can be specified using the Wyckoff (site symmetry) letter.

Figure 15: Atom dialogue.

The tool buttons of the atom dialogue allow to:

• ![Clipboard](image): transfer the dialogue to the clipboard.
• ![AFF Tables](image): display the AFF tables (Fig. 16).\(^5\), \(^6\), \(^7\), \(^8\)
• ![Help File](image): display a help file.

---


\(^7\)L. Peng et al. (PRDW), Acta Cryst.**A52** (1996) 257.

4.5 Crystal builder → Space-group dialogue

The Space-group dialogue (Fig. 17) defines the space-group and lattice parameters of an orthorhombic unit cell. The conventional and non-conventional space-groups are organised by crystal system (from triclinic to cubic). The table of the conventional orthorhombic system displays also the lattice parameters' controls and the non-conventional one the alternate groups that depend on the permutation of the a, b, c lattice parameters.
The tool buttons of the space-group dialogue allow to:

- : transfer the dialogue to the clipboard.
- : display the space-group general and special positions as well as its point-group (Fig. 13a).
- : display a help file.

### 4.6 Regular Point System code dialogue

The symmetry operations of the space-group and the lattice parameters are also entered using the RPS code dialogue (menu item *Crystal → System → RPS code* or tool button only available from the main jems window (Fig. 18) \(^9\).

The tool buttons of the RPS code dialogue allow to:

- : print the RPS code table.
- : save the RPS code table.
- : transfer the dialogue frame to the clipboard.

\(^9\)It is always simpler to define the space-group using the space-group dialogue since special positions (site symmetry, i.e. Wyckoff letter) allow a safer and faster setting of the fractional coordinates of the atoms position.
Figure 18: RPS code dialogue for entering the regular point system code.

- • : display the space-group general positions as well as its point-group when identified (Figs 13a, 13c).
- • : display a help file.

This dialogue permits to define pretty strange unit cells since the validity of the RPS code for a given crystal system is not checked (Fig. 19).

The tool buttons of the RPS code table allow to:

- • : add a new RPS code.
- • : delete the selected RPS code.
- • : erase all RPS codes (except \((x, y, z)\)).
The tool button opens the RPS code editor dialogue (Fig. 19a). The adds a new code and closes the dialogue and update the list of RPS codes (Fig. 19b). The modified unit cell can be a bit unusual since jems does not check the validity of the new RPS code (Fig. 19c). Nevertheless the RPS code editor is useful to define similar unit cells of different crystal systems. 

(a) RPS code editor dialogue. (b) Using the Editor keys (or entering the code directly) to define a new code (x, y + 1/4, z - 1/2). (c) jems does not check the new code validity → 3-D view of the updated unit-cell.

Figure 19: RPS code editor.

---

10For example in case of phase transformation.
Figure 20: ZnTe perspective view.
5.1 Popup menu

The popup menu (Fig. 165) associated with the view allows to transfer the view to the clipboard as well as to save, print, create a Mathematica notebook or generate a powder pattern. It controls also the creation of the movies.

5.2 Tool buttons

The tool buttons allow to:

- : print the table.
- : save the table.
- : transfer the frame to the clipboard.
- : open the Specimen dialogue (Fig. 88a).
- : display a Powder pattern (Fig. 120).
- : duplicate the unit cell \( n_x \times n_y \times n_z \) (Fig. 166b).
- : display a help file.

Figure 21: 3-D view popup menu.
5.3 Tabs

3-D view controls are collected in the following tabs in order to define:

- **Atoms**: the atoms colour and size as well as bonding and resolution (Fig. 167a).
- **Direction**: the viewing direction (Fig. 167b).
- **Display**: the 3-D perspective details (Fig. 167c).
- **Duplicate**: the model duplication (Fig. 167d).
- **View**: the view type (Fig. 167e).
Figure 23: Controls of 3D-perspective.

The **Atoms** and **Display** tabs are organized in sub-tabs that control the colour and size of the atoms as well as the bonding and resolution of the views (Figs. 168a, 168b, 168c, 168d, 168e, 168f, 168g, 168h). They allow, for example, to create **Black & White** figure (169a) or to look at (hkl) planes (Fig. 169b).
(a) Zn colour and size.
(b) Te colour and size.
(c) Define the bonding of ZnTe.
(d) Resolution of the spheres and bonds.

(e) 3D-view details.
(f) Cut thickness and distance to middle of model (when Cut check-box is selected).
(g) Movie controls.
(h) Cut plane selection (when Cut check-box is selected).

Figure 24: Atoms and Display Tabs.
Figure 25: Modified 3-D views.
6 SAED patterns

Plotting Selected Area Electron Diffraction patterns (SAED) is activated by either the **Drawing → Diffraction** menu item or the tool button 🖼️. The SAED frame (Fig. 26) shows the SAED pattern of the crystal structure shown in (Fig. 1) along the selected [uvw] zone axis.

![SAED patterns frame](image)

**Figure 26:** SAED patterns frame.

6.1 Tool buttons

The tool buttons of the SAED frame allow to:

- 🖨️: print the SAED pattern.
- 📖: save the SAED pattern.
- 🖇️: transfer the frame to the clipboard.
- 📠: load an experimental SAED pattern.
• • : move the Center of the Laue Circle (CLC) down.
• ↑ : move the CLC up.
• ← : move the CLC left.
• → : move the CLC right.
• # : reset the CLC to (0,0,0) reflection.
• ▼ : search the closest zone axis.
• ● : open the Microscope dialogue (Fig. 112).
• ⌂ : open the Specimen dialogue (Fig. 88a).
• ◀ : start/stop the precession mode.
• ⌚ : start/stop magnifying the experimental SAED pattern (Fig. 27).
• □ : tabulate the plotted reflections (Fig. 28).
• 🔍 : open the Keeper dialogue (Fig. 94).
• 🔍 : open the associated help dialogue.
Figure 27: Experimental SAED with a magnified area (yellow square).
6.2 Tabs

All the controls necessary to draw SAED patterns are grouped in tabs that contains controls to:

- **Avalanche**: allows selecting a single or a range of \([u,v,w]\) zone axis directions to plot, print or save as a .pdf booklet (Fig. 29a).

- **Crystal / matrix**: change the crystal thickness, perform dynamical calculations (Bloch-wave approach), select the Laue zones to plot or change the foil normal and zone axis (Fig. 29b).

- **Diffraction**: change the acceptance angle, the camera length, the calibration, the beam convergence, the deviation (number of reflections) and the accelerating voltage (Fig. 29c).

- **Lattice**: change the lattice parameters (Fig. 29d).

- **Laue zones**: boost the reflections intensity of the Laue zones (Fig. 29e).

- **Options**: select plot options (i.e. background, colour, etc) (Fig. 29f).

- **Orientation**: set the relative orientation of the experimental and calculated patterns (Fig. 30a).
- **Process**: perform some image processing operations on the loaded experimental SAED pattern (Fig. 30b).

- **Variant**: plot epitaxial or twinned patterns (Fig. 30c).

---

**Figure 29: First 6 tabs of SAED plotting controls.**

---

\(^{11}\)Only available when an experimental SAED pattern is loaded.
6.3 Popup menu

The popup menu attached to the SAED drawing duplicates several options of the Options tab (Fig. 31a).

Popup menu item Move center when selected allows to move the center of the diffraction pattern by dragging the green cross. When unselected the CLC is moved (also dragging the green cross), and the crystal is tilted away from the \([u, v, w]\) zone axis direction\(^{12}\). The blue cross marks the diffraction pattern center, i.e. the center of the \((0, 0, 0)\) reflection.

\(^{12}\)The crystal orientation is always defined by the \([u, v, w]\) zone axis indices and the \((h, k, l)\) of the CLC, the CLC being the projection of the Ewald center on the Zeroth Order Laue Zone (ZOLZ).
(a) SAED popup menu → Move center selected.

(b) SAED drawing with HOLZ reflections and lines.

(c) SAED drawing with HOLZ reflections and lines.

(d) SAED drawing with HOLZ reflections and lines and Laue circles.

Figure 31

Popup menu item **Show HOLZ lines** displays the First Order Laue Zone (FOLZ) reflections and corresponding lines of the \((0, 0, 0)\) reflection zoomed 10 times. A mouse click on any HOLZ line highlights in red the HOLZ line and its associated reflection (Fig. 31b).

Popup menu item **Scale** \([\text{mrad}]\) when selected defines the scale in \([\text{mrad}]\) instead of \([\text{nm}^{-1}]\) (Fig. 31c).
Popup menu item **Show Laue circles** when selected displays the Laue circles (Fig. 31d).

Popup menu item **Show Kikuchi lines** when selected displays the Kikuchi lines.

Popup menu item **Show SAED pattern** opens a frame with a SAED pattern image (Fig. 32a) and a 3-D view can be created using the popup menu attached to the image (Fig. 32b).

![SAED image](image1.png) ![SAED 3-D view](image2.png)

(a) SAED image (intensity log scale, FOLZ reflections intensity x 100). (b) SAED 3-D view.

Figure 32: SAED images

### 6.4 Sliders of Diffraction tab

Sliders in jems allow to modify parameters of drawings and images. Most sliders have a popup menu of type shown on Fig. 33a. The **Live** check box when selected forces the slider to update immediately the drawing or image. When unselected the update happens when the pointer leaves the slider. For lengthy updates it is good practice to unselect it. The **Fine** check box decreases the range of the slider. It is always possible to enter directly a value (within the selected range). Hit the **Return** keyboard key to confirm the entered value.

Sliders of parameters provided in [nm$^{-1}$] can be modified to accept values in [mrad] (Figs 33b, 33c).
6.5 Other SAED parameters

Check boxes of Fig. 34a allow keeping constant a selection of drawing parameters when changing crystal structure or \([u, v, w]\) zone axis direction.
The source of the Atomic Form Factors (AFF) is selected using the radio buttons of Fig. 34b. The source is described by a little tip text.

(a) Check boxes fixing selected parameters.

(b) Radio buttons selecting the AFF source.

Figure 34: SAED 2-D image and 3-D view.

6.6 SAED Bloch-wave calculation

The reflections intensity can be calculated when multiple scattering effects are included (dynamical calculation). This can be done either in the 2-beams approximation or all beams condition with or without HOLZ reflections included (Fig. 35). The calculation accepts a few hundred reflections and the intensity of the reflections is tabulated for thicknesses up to 500 nm. Remember that the calculation time is proportional to the third power of the number \( n \) of reflections \((n^3)\). The number of reflections is selected using the Deviation slider that includes reflections at a distance to the Ewald sphere smaller than "Deviation" (Fig. 33c).

The Start button starts the dynamical calculation and the Crystal thickness slider changes the crystal thickness. A mouse click on a \((h,k,l)\) reflection (except \((0,0,0)\)) displays its intensity and phase (modulo \(2\pi\)) as a function of crystal thickness (Fig. ??). Mathematica tables and plots can then be created as well as text files (Figs 37a, 37b).
Figure 35: Dynamical SAED calculation controls.

Figure 36: Plot of the intensity/phase of reflections as a function of crystal thickness.
Figure 37: Mathematica plots of the (0, 1, 0) reflection intensity and phase (modulo 2\pi).

6.7 SAED precession calculation

SAED precession calculations are performed by first tilting the crystal a few degrees out of perfect zone axis direction and then starting the precession using the tool button. The deviation should be set to a low value (\sim 0.1 [nm^{-1}]) since all the reflections are put into Bragg conditions during the precession. Precession calculations that include multiple scattering (dynamical diffraction) are performed using Imaging \rightarrow Bloch-wave \rightarrow CBED (sec. ??).
Figure 38: SAED precession settings, camera length 2000 [mm], deviation 0.1 [nm$^{-1}$], tilt 3.0 [deg].

(a) SAED precession rotation, ZOLZ & FOLZ.

(b) Precession image (log scale).

Figure 39: SAED precession.
7 Bloch-wave calculations

Bloch-wave calculations is activated by Imaging → Bloch-wave menu item. The Bloch-wave frame (Fig. 40) allows to calculate CBED, LACBED and HREM images.

![Figure 40: Bloch-wave calculations frame.](image)

7.1 Tool buttons

The tool buttons of the Bloch-wave frame allow to:

- Print: print the plot or image.
- Save: save the crystal structure in .txt format.
- Transfer: transfer a frame image to the clipboard.
- Default: set the default gray LUT.
- Microscope: open the Microscope dialogue (Fig. 112).
- Apertures: open the Apertures dialogue (Fig. 83).
• Open the Wave-front aberrations dialogue (Fig. ??).
• Control the holography biprism (when holography mode is enabled).
• Open the Specimen dialogue (Fig. 88a).
• Open the Transfer function frame (Fig. 101).
• Start/stop the SAED precession.
• Tabulate the \((h,k,l)\) reflections (Fig. 41).
• Open the toolbox with context dependent controls.
• Open the Keeper dialogue (Fig. 94).
• Reset the wave-front aberrations and imaging conditions.
• Open the associated help dialogue.

![Reflections table](Figure 41: Reflections table.)
7.2 Tabs

The controls of the parameters for the different Bloch-wave calculations are grouped in the following tabs in order to calculate:

- **Bloch-wave**: Bloch-wave images (Fig. 42a).
- **Channeling**: channeling images (Fig. 42b).
- **CBED**: CBED, LACBED and dynamical precession patterns (Fig. 42c).
- **HREM map**: maps of HREM images (Fig. 42d).
- **Rocking curve**: rocking curves (Fig. 42e).
- **Tilt table**: tables of tilted HREM maps (Fig. 42f).

![Figure 42: Tabs of the different Bloch-wave calculations.](image-url)
7.3 HREM images map calculations using the Bloch-wave method

In order to calculate a HREM images map (Fig. 43) by the Bloch-Wave (BW) approach, it is necessary to define the:

- The image formation model. The "Coherent" model assumes a coherent illumination, "Envelope" introduces the attenuation envelopes due to partial coherence and "TCC" uses Transmission Cross Coefficients.
- Camera length [nm] and number of reflections (set using the context sensitive tool box button).
- Illumination and image formation model (Fig. 44a).
- Imaging conditions, defocus [nm] and image dimension (Figs 44c, 44d).
- Crystal thickness [nm], images map, AFF and HRTEM imager (Figs 44e, 44f, 44g, 44h).
- 2-fold astigmatism [nm], 2nd order coma [nm], 3-fold astigmatism [nm] and objective aperture diameter [nm\(^{-1}\)] (Fig. 45a).
- Defocus [nm], 3rd and 5th spherical aberrations [mm] (Fig. 45b).
- Image shift [nm] and phase shift [deg] (Fig. 45c).
- Specimen drift, Thermal Magnetic noise (TM noise) and specimen vibration (Figs 46a, 46b).

Note that the transfer function intensity is plotted on Figs 44a, 44b, 44c. The popup menu associated with the plot allows to identify the transferred spatial frequencies (Fig. 44b). The line colours are:

- **Red**: transfer function including attenuation due to partial spatial and temporal coherence as well as Thermal Magnetic noise (TM).
- **Yellow**: thermal magnetic noise.

---

13 The thickness step in HRTEM calculations by the Bloch-wave method is not necessarily a multiple of the unit cell thickness.
14 When placing the pointer (mouse) on the transfer function drawing, the defocus is modified using the keyboard arrow keys ↑ and ↓.
15 The phase shift control is active when a beam stop is inserted in the back focal plane of the objective lens (apertures dialogue).
16 The intensity plot is intended to identify the reflections transferred by the objective lens (lines are indexed when aimed).
17 Cancels the TM noise as well all other aberrations (except the spherical aberrations).
- **Green**: partial spatial coherence (beam convergence).
- **Blue**: partial temporal coherence (defocus spread).

Figure 43: $AuCu_3$ (8 × 8) HREM images map with decreasing defocus (horizontally) and increasing thickness (vertically).
(a) Illumination and imaging model.
(b) Popup menu associated with the transfer function drawing (intensity).
(c) Starting defocus (d) Defocus series [nm] (minimum), defocus size and duplication step [nm].
(e) Minimum crystal thickness [nm], number of iterations, thickness increment [nm].
(f) Plot and map options.
(g) HREM map iteration options.
(h) Reflections number and Bethe approximation.

Figure 44: Controls the illumination, defocus, specimen thickness values, number of strong reflections and introduces Bethe approximation.

When the wave-functions are saved (as .ems) images and the "Start HRTEM imager" is selected (Fig. 44g) a frame is activated that allows to introduce in the HRTEM image calculations all wave-front aberrations (up to order 8) as well as beam tilt and objective aperture center among others (??).
Figure 45

(a) Objective lens aberrations [nm] and objective aperture size [nm] - 1
(b) Defocus [nm] 3rd and 5th order spherical aberrations [nm]
(c) Image shift [nm] and phase shift [deg].

Figure 46

(a) Image drift [nm s^-1] and Thermal Magnetic noise [pm]
(b) Specimen vibration [nm].
When the MTF of the camera Modulation Transfer Function (MTF) has been measured it is possible to introduce its effect in the HRTEM image simulation. This requires to enable the Plot → Image check box (Iteration → Map → Plot → Image). When HRTEM image calculation is completed select the panel (HREM map → Plot)\(^\text{18}\) (Figs 48a, 48a, 49a, 49a).

The HRTEM imaging parameters used by the image displayed on the Plot panel can be changed interactively. As an example select the Obl. lens tab and modify the 3-fold astigmatism and its orientation (Figs 50c, 50f, 50e, 50f).

\(\text{Figure 47: Controls to introduce the camera MTF in the HRTEM simulations.}\)

\(\text{\(^\text{18}\)To start the calculation either the Diffraction or Map tab must be selected}\)
(a) At low magnification the camera transfers only low spatial image frequencies.

(b) At low magnification the contrast and resolution of the image are low.

Figure 48: Low magnification.

(a) At high magnification the camera transfers high spatial image frequencies.

(b) At high magnification the contrast and resolution of the image are high.

Figure 49: High magnification.
By default 2 MTF are listed in the MTF table:

- a camera with a constant MTF of value 1.0.
- a 1024 x 1024 camera of 24 $\mu m$ pixel size.

As an example select the **Obj. lens** tab and modify the 3-fold astigmatism and its orientation (Figs 50b, 50a, 50c, 50d, 50e, 50f).\(^{19}\)

\(^{19}\)A popup menu is associated with the image in order to transfer it to the clipboard.
(a) 3-fold astigmatism orientation control (a value is set by dragging the needle or clicking on a graduation).

(b) 3-fold astigmatism orientation control and associated popup menu. **Auto rotate** popup menu item changes continuously the orientation.

(c) 300nm 3-fold astigmatism oriented at 0°.

(d) 300nm 3-fold astigmatism oriented at 60°.

(e) 600nm 3-fold astigmatism oriented at 0°.

(f) 600nm 3-fold astigmatism oriented at 60°.

Figure 50: Effect of 3-fold astigmatism on HRTEM images.
The contrast of the plotted HRTEM image is modified using the controls provided in context specific tools boxes (Figs 51a, 51b, 51c).

(a) Tool box of **Diffraction** context to change the camera length and the number of reflections (deviation control).

(b) Tool box of **Map** context to change the image contrast.

(c) Tool box of **Plot** context to change the plotted curve (intensity versus thickness of \((h,k,l)\) reflections), the crystal thickness, and the image contrast.

Figure 51: Tool boxes of **Diffraction** (a), **Map** (b) and **Plot** (c) contexts.
7.4 CBED patterns calculation using the Bloch-wave method

Fig. 52a displays the main tab for calculating Convergent Beam Electron Diffraction (CBED) patterns. The camera length, deviation and Laue zones controls of the toolbox are activated using tool button. The convergence of the incident electron beam is set by the Beam half conv \([mrad]\) control. Its popup menu allows to set it in \([nm \text{ } – \text{ } 1]\) (Fig. 52b). The CBED defocus control makes possible to calculate coherent CBED.
(a) CBED calculation by the Bloch-wave method.

(b) Illumination control ($[nm - 1]$) set to have just touching reflections.

Figure 52: ZnTe [1, 1, 0] CBED pattern calculation.
The CBED calculations are controlled using sliders, check boxes or radio buttons distributed in the following tabs:

- **Illumination**: Figs 53a, 53b.
- **Iteration**: Figs 53c, 53d, 53e.
- **Laue zones**: Fig 53f.
- **Scan control**: Figs 54a, 54b.
- **Vhkl editor**: Fig. 54c.
(a) Beam half-conv \([mrad]\) or \([nm - 1]\) and CBED defocus \([nm]\) controls.

(b) HOLZ threshold \([mV]\) and Zoom controls.

(c) Defines the minimum thickness \([nm]\), the number of thickness steps and the increment of the steps. The thickness step minimum is 1 \(nm\).

(d) Defines CBED options to Show the progress of the calculation, scan a rectangular area instead of the circular area delimited by the \((0, 0, 0)\) spot, to fix the gamma for all the series of CBED patterns, displays the ZOLZ lines and uses a linear or logarithmic intensity scale.

(e) Sets the minimum number of the strong reflections. When the Bethe checkbox is enabled a weak reflection is selected, its effect is introduced in the calculation using the Bethe perturbation approximation.

(f) Boosts the intensity of the HOLZ reflections and lines shown on the Diffraction plot.

Figure 53: CBED controls tabs.
(a) Simulates **Hollow cone illumination**.

(b) Defines the dynamical precession parameters: rotation increment, precession angle [degree] and the size of the intensity integration area.

(c) Allows to set the structure factor of selected reflections.

Figure 54: CBED controls tabs.

(a) 80 nm, ZnTe [110]. Vertical symmetry plane is missing to ZnTe polarity (thickness and contrast settings provided by the toolbox).

(b) 80 nm, ZnTe [110], indexed reflections (using the toolbox).

(c) 80 nm, ZnTe [110], reflections are indexed & colour LUT (using the popup menu).

Figure 55: CBED patterns.
Figure 56: Tilted CBED patterns.

7.5 Large Angle CBED (LACBED)

Figure 57: LACBED patterns, (001) reflection (bright field).

7.6 CBED precession

7.7 CBED follow cone
8 Multislice calculations

Figure 58: Multislice frame.

8.1 Tool buttons

The tool buttons of the multislice frame allow to:

- Print: print the plot or image.
- Save: save the crystal structure in .txt format.
- Transfer: transfer a frame image to the clipboard.
- Set: set the default gray LUT.
- Microscope: open the microscope dialogue (Fig. 88a).
- Apertures: control the size and (h,k,l) center of the apertures (Fig. 83).
- Wave-front aberrations: open the Wave-front aberrations dialogue (Fig. 100).
- Biprism: control the holography biprism (when holography mode is enabled).
- Specimen: show the Specimen dialogue (Fig. 88a).
• : open Map, Plot, Projection tabs controls.
• : open the Transfer function frame (Fig. 101).
• : reset the wave-front aberrations and imaging conditions.
• : open the associated help dialogue.

8.2 Tabs

The controls of the parameters for the different Bloch-wave calculations are grouped in the following tabs in order to calculate:

• **Fresnel propagator**: the propagation of the wave-function from slice to slice (Fig. 59a).
• **Phase object function**: the interaction of the wave-function with a slice (Fig. 59b).
• **Projected potential**: the projected potential of a slice (Fig. 59c).
• **Absorptive potential**: the absorptive potential (Fig. 59d).
• **Atom position**: the atoms position (scaled to the projected potential size) (Fig. 59e).
• **HAADF image**: High Angle Annular Dark Field images of a stack of super-cells (Fig. 59f).
• **HREM map**: HREM images map (Fig. 59i).
• **Super-cell image**: HREM images of a stack of super-cells (Fig. 60a).
• **Nano diffraction**: CBED patterns of a stack of super-cells (Fig. 60d).
(a) Fresnel propagator between slices (4 x 4) unit cells.

(b) Phase object function of a slice (4 x 4) unit cells.

(c) Projected potential of a slice (4 x 4) unit cells.

(d) Absorptive potential of a slice (4 x 4) unit cells.

(e) Atom position in a slice (4 x 4) unit cells.

(f) HAADF image.

(g) HAADF probe dialogue.

(h) Wave-front aberrations (up to order 8).

(i) HREM image maps (2 x 2 unit cells, 4 x 4 images).

(j) HREM image maps (2 x 2 unit cells, 4 x 4 images, labelled with defocus, thickness & atomic columns position).

(k) HREM image viewed in Plot tab (using Iteration → Options → Others & Plot → Image). The thickness and contrast of the displayed image are changed using the controls appearing when the tool button is pushed.

Figure 59: Tabs of multislice calculations frame.
(a) Super-cell HRTEM images (with the camera MTF panel).
(b) Super-cell Plot tab that enables to vary imaging conditions, in particular aberrations. Thickness is set using the tool button.
(c) Super-cell model generated from the stack of cells (Cell → tool button).
(d) Nano-diffraction tab.
(e) Nano-diffraction pattern, projected model.
(f) CBED nano-diffraction calculated by the multislice method.

Figure 60: Tabs of multislice calculations frame (continued).

The images and maps dimension (width, height) are set in the Parameters → Preferences → Imaging tab, where the size of the GUI panels is also defined. Recommended typical values (depending of the PC or Laptop screen resolution) are:

- 1024 for Maximum dimension of reduced images.
- 1024 for Maximum image dimension.
- 4096 for Maximum map dimension.

The other setting that sets the HREM image dimension is the Pixel size of high resolution images \([\text{nm}]\). As an example selecting a pixel size of 0.01 \([\text{nm}]\) means that the projected potential of a \(1 \times 1 \text{[nm}^2\] unit cell will be sampled with a step size of maximum [0.01] \text{nm} and then its maximum dimension will be 128 × 128

71
pixels. For a $10 \times 10$ $[nm^2]$ super-cell the projected potential dimension will be $2048 \times 2048$ pixels. For such large cells a $0.02$ $[nm]$ pixel size is recommended (depending on the computer).

Images or maps larger than their specified maximum dimension will be reduced automatically.

8.3 HREM images map calculations using the multislice method

The HREM map controls are placed in tabs that are almost identically organised as found in the Bloch-wave HREM calculation with the exception of the Multislice $\rightarrow$ HOLZ reflections tab (Fig. 61a). Some of the controls are put in a sub-tab Multislice $\rightarrow$ Frozen lattice tab (Fig. 61b).

The Multislice offers 3 different ways to generate the projected potential of any crystal slice:

- **Analytic** analytical calculation, slightly slower than Direct.
- **Direct** atoms potential is calculated and patched at its fractional $(x, y)$ image coordinates. It is faster than Fourier or Analytic methods but can produce artefacts (eliminated with checkbox Frozen lattice $\rightarrow$ Enable which introduces lattice vibrations (Einstein model)).
- **Fourier** done in Fourier space. Most precise and most time consuming.

The HOLZ reflections can only be included in the multislice calculations when the crystal is cut into slices thinner than the unit cell thickness $^{20}$.

The **Reset** button erases the Phase Object Function (POF). The POF images can be saved for future use or loaded in order to redo a calculation.

$^{20}$Only orthogonal cells can be sliced. To create an orthogonal cell use menu item Crystal $\rightarrow$ Make orthogonal or Crystal $\rightarrow$ Transform unit cell.
(a) **Multislice → HOLZ reflections** tab controlling the generation of the projected potential of the crystal slices.

(b) **Multislice → Frozen lattice** tab controlling atom displacement and potential interpolation.

Figure 61: **HREM → Multislice** tabs.
8.4 HAADF image calculations using the multislice method

Figure 62: HAADF image calculation.
9 HRTEM imager

The HRTEM imager is shown on Fig. 63. It allows to introduce in the HRTEM image simulation wave-front aberrations up to order 8, the effects of crystal or beam tilt as well as "out of center" objective aperture or beam stop (Zernike phase contrast). The calculations are interactive, i.e. a change of any imaging parameters can be seen in real time in the Image panel. The left part of the HRTEMImager frame controls the simulation of the images and the right part displays either the HRTEM image, the Contrast Transfer Function (CTF) or the Wave-Function (WF).

Figure 63: HRTEM imager frame (activated with the largest crystal thickness).

9.1 Tool buttons

The tool buttons of the HRTEM imager allow to:

- : print the image, CTF or wave-function.
- : save the image, CTF or wave-function
• [Transfer HRTEM frame to clipboard.]
• [Open a wave-function (.ems file).]
• [Set the default gray LUT.]
• [Open the Microscope dialogue (Fig. 112).]
• [Open the Keeper dialogue (Fig. 94).]
• [Reset the aberrations.]
• [Open the associated help dialogue.]
(a) Image tab (the image is displayed as $10 \times 10\ AuCu_3$ unit cells).

(b) CTF tab (imaginary part of the transfer function).

(c) Tab displaying the "Phase" of the wave-function.

Figure 64: HRTEM imager, right tabs.
9.2 Tabs

The imaging controls are organised in several tabs aimed at:

- **Camera MTF**: introducing the camera MTF (Figs 47a, 47b), see sec. 7.3.
- **Aberrations**: including aberrations up to order 8 in the image simulation\(^{21}\) (Figs. 65a, 65b)\(^{22}\).
- **CLC selector**: controlling to tilt the incident beam (green cross), to set the reflection number and specimen thickness\(^{23}\) (Figs 65c, 65d).
- **Coherence**: changing the coherence of the illumination (65e).
- **Dark field**: setting dark field condition, i.e. move the (0,0,0) reflection away from the optical axis of objective lens (Figs 66a, 66b).
- **Defocus**: setting the defocus\(^{24}\) (Fig. 66c).
- **Defocus series**: generating series of defocused images (to be saved as .ems or .jpg and a little .html page)\(^{25}\) (Fig. 66d).
- **Drift & Noise**: introducing image specimen drift and poisson noise (Fig. 67a).
- **Holography**: generating HRTEM hologram images (Figs 67c), 67d).
- **Imaging**: adjusting image brightness, contrast, gamma as well as image tiling x & y and noise level (67f).
- **Objective aperture**: defining the size and position of the objective aperture as well as the beam stop size and phase shift to simulate Zernike phase contrast (Figs 68a, 68b)\(^{26}\).

\(^{21}\)The maximum aberration order is defined in Parameters → Preferences → Imaging → Others tab.

\(^{22}\)The label of the spherical aberration refers to the geometric aberration notation \(C_{30}\) (Krivaneck) or \(C_3\) (Haider) and the wave-front aberration \(W_{40}\).

\(^{23}\)The crystal thickness can only be modified interactively when the wave-function has been calculated by the Bloch-wave approach. When the multislice approach has been employed it is necessary to load the wave-function.

\(^{24}\)When placing the pointer (mouse) on the transfer function drawing, the defocus is modified using the keyboard arrow keys ↑ and ↓.

\(^{25}\)The defocus series can be loaded and imaged using menu item Imaging → Load → Stack.

\(^{26}\)The Stretch option increases the image contrast.
(a) Aberrations are defined using sliders.

(b) Table of aberrations with Krivanek, Haider and wave-front notations.

(c) CLC, deviation (reflections number) and crystal thickness settings.

(d) Tilted crystal (i.e. CLC \((h,k,l)\) indices set by the green cross position).

(e) Illumination coherence.

Figure 65: Aberrations, CLC and Coherence tabs.
(a) Dark field condition.

(b) CTF in dark field condition.

(c) Defocus setting.

(d) Defocus series can be saved in .ems or .jpg format.

Figure 66: Dark field, Defocus and Defocus series tabs.
(a) Drift & Noise.

(b) Vibration.

(c) Biprism voltage and orientation.

(d) HRTEM image in holography mode.

(e) Diffractogram of holography HRTEM image in holography mode.

(f) Image brightness, contrast, gamma as well as tiling and poisson noise level.

Figure 67: Drift/Noise, Holography and Imaging tabs.
(a) Objective aperture diameter $[nm^{-1}]$.

(b) Beam stop $[nm^{-1}]$ for Zernike phase contrast imaging (??).

Figure 68: **Objective aperture and beam stop & phase shift [deg] tabs.**

The wave-front aberration $W_{ij}$ defines the $i^{th}$ power of the radial angle and the $j^{fold}$ azimutal angle $^{27}$.

$^{27}$The chromatic aberration is $W_{00}$. 
9.3 Zernike phase contrast

(a) HRTEM imager allows to move, resize the objective aperture or the beam stop and shift the blocked reflection(s) interactively.

Figure 69: HRTEM imager, objective aperture settings.
Figure 70: Zernike phase contrast with out of axis objective aperture and a beam stop that phase shifts the transmitted beam and \{100\} reflections.
(a) HRTEM imager allows to move, resize the objective aperture or the beam stop and shift the blocked reflection(s) interactively.

Figure 71: HRTEM imager, objective aperture settings.
10 HRSTEM imager

![HRSTEM imager](image)

Figure 72: HRSTEM imager.

10.1 Tool buttons

The tool buttons allow to:

- ![print](image) : print the HAADF image.
- ![save](image) : save the HAADF image.
- ![transfer](image) : transfer the dialogue to the clipboard.
- ![open](image) : open a saved multislice HAADF intensity image (*xxxSTEM_nnnn.ems*).
- ![set](image) : set the default gray LUT.
- ![open](image) : open the *Microscope* dialogue (Fig. 112).
- ![open](image) : open the *Keeper* dialogue (Fig. 94).
- ![reset](image) : reset the wave-front aberrations and imaging conditions.
- ![display](image) : display a help file.
### 10.2 Controls and images tabs

The controls tabs allow to:

- **Aberrations**: change the aberrations of the probe intensity (Figs 73a, 73b).
- **Coherence**: change the coherence of the illumination (Fig. 73c).
- **Drift & Noise**: introduce probe drift or vibration & thermal magnetic noise (Fig. 73d).
- **Imaging**: duplicate the HAADF or object intensity image and modify their contrast (Fig. 73e).
- **Microscope**: modify the microscope parameters (Fig. 73f).

![Image](image1.png)

![Image](image2.png)

![Image](image3.png)

(a) Aberrations settings (table view).
(b) Aberrations settings (slider controls).
(c) Illumination coherence settings.
(d) Drift & Noise settings.
(e) Imaging settings.
(f) Microscope settings.

Figure 73: HRSTEM imager controls.

The images tabs allow to display:

- **HAADF image**: the HAADF image (Figs 74a).
• **Probe**: the probe intensity (Fig. 74b).
• **Intensity**: the object intensity (Fig. 74c).

(a) HAADF image obtained by convolution of the probe intensity with the object intensity.

(b) Probe intensity.

(c) Object intensity.

Figure 74: HRSTEM imager (**HAADF image, Probe & Intensity** tabs)

Any aberration up to wave-front aberration order 8 ($W_{80}$ to $W_{88}$) is introduced interactively using the controls of the **Aberrations** tab, for example 3-fold astigmatism (Fig. 75).

(a) HAADF image obtained by convolution of the probe intensity with the object intensity.

(b) HAADF image (inversed contrast).

(c) Probe intensity.

Figure 75: Introducing 3-fold astigmatism.
The coherence of the illumination is controlled using the Coherence tab and the Microscope tab allows to change the virtual source size (Fig. 76).

![Image](image_url)

(a) Source size 20 [pm].  
(b) HAADF image.  
(c) Probe intensity. 

(d) Source size 100 [pm].  
(e) HAADF image.  
(f) Probe intensity.

Figure 76: Effect of source size change.

The tiling of the HAADF image and object intensity is controlled using the Imaging tab (Fig. ??).
Figure 77: Imaging x & y image-tiling.
11 Camera MTF

The measurement of the camera Modulation Transfer Function (MTF) requires to load several images of the camera noise pattern (Fig. 78). This procedure measures what is called the Noise Transfer Function. Noise images of the CCD camera are acquired, i.e. images obtained without a specimen and with an illumination as uniform as possible (typically 10 noise images) (Fig. 81a). The images are then subtracted one by one at a time in order to cancel the non-uniformity of the illumination. A diffractogram is calculated and rotationally averaged to obtain the NTF profile which is finally fitted using a mathematical expression (exponential, gaussian, lorentzian or a mixed formula). The NTF usually over evaluates the MTF.

![Camera MTF frame](image)

Figure 78: Camera MTF frame.

11.1 Tool buttons

The crystal builder tool buttons allow to:

- : print the fitting drawing.
- : save the fitting drawing.
• ![Clipboard] : transfer the frame to the clipboard.
• ![Image] : open a noise pattern image (Fig. 80a).
• ![Start] : start the fitting procedure (requires at least 2 images).
• ![Table] : display a table of the fitted function and the fitted parameters (Fig. 80b).
• ![Help] : display a help file.

### 11.2 Tabs

The camera MTF frame is separated in 2 panels, the left one is used to follow the MTF fitting and the right one shows the NTF images and the selection of the fitting MTF model (Fig. 79).

![Crystal MTF → tabs](image)

(a) Table of noise images, (b) Camera normalized parameters of fitting procedure, (c) Camera PSF.

Figure 79: Crystal MTF → tabs.

The noise pattern images should ideally be acquired with a camera saturation $\sim 2/3$, typically 6'000 to 8'000 counts for the MSC Gatan CCD camera (24 $\mu$m, 1024 $\times$ 1024 pixels). The dialogue loading **Gatan data only** images requires to specify the dimension of the images, the data offset as well as the pixel type (Fig.
Fig. 81a shows a noise image. Its diffractogram (Fig. 81b) and a few profiles taken across the diffractogram that show the non-uniformity of the illumination (Fig. 81c). The Dirac delta function observed at the center of the diffractogram is not taken into account during the MTF fitting, the domain of of fitting being limited by the movable yellow lines of Fig. 78.

(a) Gatan data only images 1024 × 1024 unsigned short image format.  
(b) Experimental MTF values & fitted function as a function of the image frequency.

Figure 80: Data only load dialogue and fitted parameters table.

(a) CCD camera noise image.  
(b) Diffractogram of noise image.  
(c) Profiles across the center of diffractogram.

Figure 81: 1024 × 1024 Gatan CCD camera noise, diffractogram, profiles.

The experimental and fitted normalized NTF are plotted on Fig. 82. The maximum image frequency is the Nyquist frequency, 511 for 1024 × 1024 sized images.
Figure 82: Mathematica normalized NTF plots.
12 Apertures dialogue

12.1 Tool buttons

The tool buttons allow to:

-  
  : transfer the dialogue to the clipboard.

-  
  : display a help file.

Figure 83: Apertures dialogue.
Figure 84: Objective aperture dialogue tabs.

(a) Beam stop (Zernike phase contrast).
(b) Optical axis settings.
(c) Large Angle Convergent Beam Diffraction (LACBED) or Dark Field (DF) aperture.

Figure 85: HRTEM images with different objective aperture settings.
Figure 86: Effect of the optical axis shift (not to be confused with a crystal tilt).

(a) Optical axis centered (0, 0, 0).

(b) Optical axis shifted to (6, 4, 0).

(c) Optical axis on axis (at (000)).

(d) Optical axis at (220).
(a) Acceptance angle and camera length.

(b) Beam convergence and deviation.

(c) SAED or LACBED aperture on axis.

(d) SAED or LACBED aperture off axis.

Figure 87
13 Specimen

The specimen dialogue sets parameters related to the orientation of the thin crystal slice with respect to the optical axis of the microscope ([uvw] zone axis indices and (hkl) indices of the center of the Laue circle) as well as the number of Laue zones and the deviation, i.e. maximum distance of a (hkl) reciprocal node to the Ewald sphere.

13.1 Tool buttons

The tool buttons allow to:

- : transfer the dialogue to the clipboard.
- : open the keeper dialogue (Fig. 94).
- : display a help file.

(a) Specimen dialogue, [uvw] zone axis selection (default).

(b) [uvw] zone axis selection with less choice.

Figure 88: Use the arrows tool buttons to decrease/increase the number of plotted zone axis. [uvw] zone indices can be entered directly (keyboard return key to confirm).
(a) Default CLC is setting (000).

(b) CLC moved to (8, 4, 0) → crystal tilt 1.63 [deg]

Figure 89: Use the arrows tool buttons to move the Center of the Laue Circle (CLC).
(a) Small deviation → small number of reflections.

(b) Large deviation → large number of reflections.

Figure 90: The deviation slider defines the maximum distance of a reflection to the Ewald sphere.
(a) Foil normale is parallel to the zone axis by default.

(b) Foil normale set to \([1, 1, 2] \rightarrow \text{tilt } 35.3 \ [\text{deg}].\)

Figure 91: The foil normale sets the angle of the normale to the entrance surface of the tilted foil.

(a) Default is only \textbf{Zeroth Order Laue Zone.}\n
(b) \textbf{First Order Laue Zone.}\n
Figure 92: The arrow tool buttons increase/decrease the number of Laue zones.

102
Figure 93
14 Keeper dialogue

The Keeper dialogue keeps most jems parameters.

The Keeper dialogue allows to keep the set of parameters defined for the simulations. The crystal path is set using the crystal path button.

14.1 Tool buttons

The tool buttons allow to:

- open a set of parameters stored in a keeper file.
- save the current parameters in a keeper file.
The Aberrations tabs keep the wave-front aberrations $W_{ij}$, where $i$ denotes the power of radial aberration angle and $j$-fold azimuthal angle. In this notation only even $i$ or $j$ indices are permitted. The labels are also given in the equivalent geometric aberrations notation as defined by Krivanek $C_{ij}$ and Haider $C_c, I, Z, A_1, ...$ (Fig. 95) \(^{28}\).

(a) Wave-front aberrations $W_{00} \rightarrow W_{55}$.

(b) Wave-front aberrations $W_{60} \rightarrow W_{88}$.

Figure 95: Wave-front aberrations defined to order 8.

The 3 tabs of Fig. 96 keep parameters related to ADF, HRTEM and SAED diffraction \(^{29}\).

---

\(^{28}\)Wave-front aberration $W_{00}$ is the chromatic aberration, i.e. the aberration that only dependent on the wavelength.

\(^{29}\)The sign of the under-defocus is defined in the Parameters $\rightarrow$ Preferences $\rightarrow$ Imaging $\rightarrow$ Others.
(a) BF, annular dark field and HAADF detector diameters.

(b) Diffraction parameters.

(c) Defocus step, size of defocus series, image duplication and Poisson noise.

Figure 96: ADF imager, Diffraction and Imaging tabs.

The 3 tabs keeping parameters related to diffraction patterns indexing are shown on Fig. 97, the 3 tabs keeping the Bloch-wave and multislice iterations parameters on 98 and the 3 tabs keeping the microscope, precession, vibration and drift parameters on Fig. 99.

(a) Kikuchi indexing parameters.

(b) Spot indexing parameters.

(c) Parameters related to rotation and powder ring pattern center.

Figure 97: Kikuchi and SAED patterns indexing.
(a) Parameters of Bloch-wave calculations.  
(b) Parameters of CBED calculations.  
(c) Parameters of multislice calculations.

Figure 98: Parameters related to Bloch-wave and multislice calculations.

(a) Microscope parameters.  
(b) Precession radial angle and azimuthal increment.  
(c) Vibration and drift imaging parameters.

Figure 99: Microscope, precession and vibration parameters.
15  Wave-front aberrations dialogue

Figure 100: Wave-front aberration and Contrast Transfer Function.

15.1 Tool buttons

The tool buttons allow to:

- ![ ]: transfer the dialogue to the clipboard.
- ![ ]: open the keeper dialogue (Fig. 94).
- ![ ]: display a help file.
16  Transfer function

Figure 101: Wave-front aberrations.

16.1  Tool buttons

The tool buttons allow to:

- : print the image panel.
- : save the image panel.
- : transfer the frame to the clipboard.
- : reset the gray scale.
- : open the Microscope dialogue (Fig. 112).
- : make a tilt tableau (Fig. 109).
- : open the Specimen dialogue (Fig. 88a).
- : tabulate the image panel.
- : open the Keeper dialogue (Fig. 94).
(a) CTF profile tab (with envelopes and ZnTe powder lines).

(b) CTF 2-D tab.

Figure 102: Contrast Transfer Function (CTF).
(a) Diffractogram tab (amorphous carbon thin film).

(b) OTF tab.

Figure 103: Diffractogram and Optical Transfer Function.

(a) Probe shape tab (intensity).

(b) Ronchigram tab.

Figure 104: Probe shape and Ronchigram.
(a) Aberration settings tab.  
(b) Coherence settings tab.

Figure 105: Aberrations and coherence settings.

(a)  
(b) 

Figure 106: Defocus and drift or noise settings.
Figure 107: Microscope and shift or tilt settings.
(a) Table of aberrations, $w_{44} = 4 \, [\mu m]$.  
(b) Wave-front aberrations ($w_{44} = 4 \, [\mu m]$).  
(c) Aberrated CTF profile ($w_{44} = 4 \, [\mu m]$).

(d) CTF 2-D ($w_{44} = 4 \, [\mu m]$).  
(e) Diffractogram ($w_{44} = 4 \, [\mu m]$).  
(f) Ronchigram ($w_{44} = 4 \, [\mu m]$).

Figure 108: Wave-front aberrations, CTF, diffractogram and Ronchigram with 4-fold astigmatism $4 \, [\mu m]$. 

114
Figure 109: Tilt tableau no aberrations, tilt amplitude 2 [mrad].

Figure 110: Tilt tableau 3-fold astigmatism, tilt amplitude 2 [mrad].
Figure 111: Tilt tableau, 3-fold astigmatism and tilted illumination 2 [mrad].

(a) Tilted illumination 2 [mrad].

(b) Tilt tableau, 3-fold astigmatism 800 [nm], 60 [deg], illumination tilt 2 [mrad].
17 Microscope dialogue

Figure 112: Microscope dialogue.

17.1 Tool buttons

The tool buttons allow to:

- ![Load](image) : load a microscope table.
- ![Save](image) : save the table of microscopes.
- ![Transfer](image) : transfer the frame to the clipboard.
- ![Add](image) : add a new microscope.
- ![Delete](image) : delete the selected microscope.
- ![Default](image) : load the default microscope table.
• : open the specimen dialogue (Fig. 88a).
• : display a help file.

The plot of Fig. 113b shows the intensity of the Contrast Transfer Function with positive sign for the underfocus. The Parameters → Preferences → Imaging → Others tab allows to use the opposite sign.

The yellow envelope introduces the effect of Thermal Magnetic Noise that can attenuate the CTF of aberrations corrected microscopes.

(a) Tab to control partial temporal and spatial coherence.

(b) CTF intensity plot.

Figure 113: CTF plot (positive underfocus).
18 Crystallographic calculator

Figure 114: Crystallographic calculator.

18.1 Tool buttons

The tool buttons allow to:

- ![print](button) : print the frame.
- ![save](button) : save the frame.
- ![clipboard](button) : transfer the frame to the clipboard.
- ![help](button) : display a help file.

The crystallographic calculator performs several calculations related to direct or reciprocal space. Fig. 114 shows a typical calculation of the angle between 2 zone axis directions ([2, 3, 0] & [2, 3, 5]). It also shows the orthogonal cell with [0, 0, 1] parallel to [2, 3, 0] (Fig. 115a). When the calculation is performed with 2 \((h, k, l)\) reflections the SAED pattern defined by them is shown (Fig. 115b) \(^{30}\).

\(^{30}\)When the calculations are first performed with \(<uvw>\) directions, the following calculations with \{hkl\} reflections use the new unit orthogonal unit cell. (Figs. 115c, 115d)
(a) Orthogonal cell with \([0, 0, 1]\) parallel to \([2, 3, 0]\).

(b) SAED pattern defined by \((2, 3, 0)\) and \((2, 3, 5)\) reflections.

(c) SAED pattern defined by \((2, 3, 0)\) and \((2, 3, 5)\) reflections. The **not saved** label indicates that the \(2 (hkl)\) reflections refer to the new orthogonal cell.

(d) SAED pattern defined by \((1, 0, 0)\) and \((0, 1, 0)\) reflections, i.e. the \([2, 3, 0]\) SAED pattern from \(AuCu_3\) unit cell.

Figure 115: Crystallographic calculator SAED plots with the orthogonal cell.
(a) Popup menu attached to the SAED pattern.

(b) SAED pattern with Kikuchi lines.

Figure 116: Popup menu and Kikuchi lines.
19  Stereogram frame

Figure 117: Stereogram frame.
19.1 Tool buttons

The tool buttons allow to:

- : print the stereographic projection.
- : save the stereographic projection.
- : transfer the frame to the clipboard.
• ✖️: overlay stereograms.
• ✗️: make a table of zone axis.
• 🔧: open the toolbox.
• 📚: display a help file.
19.2 Tabs

(a) Indexed \{hkl\} stereogram.

(b) Indexed \langle uvw \rangle stereogram.

(c) Superposed \{hkl\} and \langle uvw \rangle stereograms.

(d) Wulff net.

Figure 119: Stereogram tabs.
20 Powder pattern frame

![Figure 120: Powder pattern frame.](image)

20.1 Tool buttons

The tool buttons allow to:

- ![ ]: print the stereogram.
- ![ ]: save the stereogram image.
- ![ ]: transfer the frame to the clipboard.
- ![ ]: display a help file.

The powder pattern plots only show the lines position and intensity (Fig. 120). The parameters of the different radiations are gathered in the 3 tabs on the right panel. Controls to plot neutron and X-Ray powder patterns allows to change the wavelength of the radiation (Figs 121a, 121b). The horizontal axis unit can be either degree or $nm^{-1}$ (Figs 122a, 122b).
(a) Controls for neutron powder pattern plots.

(b) Controls for X-Ray powder pattern plots.

Figure 121: Tabs of Neutron and X-Ray powder pattern controls.

(a) Electron powder pattern and popup menu to switch horizontal axis unit from degree to \( nm^{-1} \).

(b) X-Ray powder pattern with indexed reflections and \( nm^{-1} \) unit (Co \( K_{\alpha1} \) source).

Figure 122: Electron and X-Ray powder patterns.
21 Zone axis geometry frame

Figure 123: Table of zone axis geometry for indexing SAED patterns.

21.1 Tool buttons

The tool buttons allow to:

- : print the zone axis table.
- : save the zone axis table.
- : transfer the frame to the clipboard.
• 📚 : open another crystal and create and add a zone axis table.
• 🔍 : index a SAED pattern using the table(s).
• 🎨 : display a help file.
22 Transform unit cell dialogue

![Figure 124: Transform unit cell dialogue.](image)

22.1 Tool buttons

The tool buttons allow to:

- 📐: print the dialogue.
- 📈: save the dialogue image.
- ☀️: transfer the dialogue to the clipboard.
• select a unit cell transformation (Fig. 125a).
• show the transform unit cell (Fig. 125b).
• display a help file.

(a) Table of unit cell transforms. (b) 3-D view of transformed unit cell.

Figure 125: $AuCu_3$ transformed unit cell.
23 Make orthogonal dialogue

The left table shows the unit cell parameters and atoms position of the original cell. The orthogonal cell parameters and atoms position are shown on the right table. The orthogonal cell [0, 0, 1] direction is parallel to ZnTe [1, 2, 1] direction, its [1, 0, 0] and [0, 1, 0] directions are parallel to the ZnTe [1, −1, 1] and [1, 0, −1] directions. Its volume is 6 times the volume of the ZnTe unit cell. The orthogonal cell can be pretty large depending on the \(uvw\) direction (Fig. 128) \(^{31}\).

23.1 Tool buttons

The tool buttons allow to:

- ☑️: print the frame.
- ☐️: save the frame.
- ☐️: transfer the frame to the clipboard.
- ☑️: open the specimen dialogue (Fig. 88a).
- ☑️: show the orthogonal unit cell (Fig. 127).
- ☑️: display a help file.

\(^{31}\)The lattice angles are still 90° though they can be slightly lower depending on the original unit cell.
Figure 126: Dialogue to create orthogonal cells.
Figure 127: Orthogonal cell with [0, 0, 1] parallel to ZnTe [1, 2, 1] direction.
(a) Orthogonal cell parameters and atoms position with [0, 0, 1] parallel to ZnTe [2, 5, 1] direction.

(b) Orthogonal cell 3-D view with [0, 0, 1] parallel to ZnTe [1, 2, 1] direction.

Figure 128: ZnTe [2, 5, 1] orthogonal cell contains 240 atoms (8 × 30).
Figure 129: Image processing frame with experimental GaN HRTEM image loaded.
Figure 130: Table of image pixels.

Fig. 131 show a few examples of processing an experimental HRTEM image.
Figure 131: Image processing of Si [100] HRTEM image (FEI CM-300).

24.1 Tool buttons

The tool buttons allow to:

- 📹: print the image.
- 📖: save the image.
• : transfer the frame to the clipboard.
• : open an image.
• : tabulate the image (Fig. 130).
• : select and cut part of image.
• : apply selected process (Fig. 133b).
• : Fourier transform part of image.
• : show 3-D view.
• : magnify part of image.
• : open the toolbox.
• : display a help file.
24.2 Tabs

(a) Histograms tab that displays the image histogram before and after processing.

(b) Options tab that controls image contrast options and magnifier zoom.

Figure 132: Image processing tabs.
24.3 Example

The image processing tab is available in several jems frame. It can be used to automatically identify the center of spots on diffraction patterns (Fig. 134).

Figure 133: Image processing tabs.
(a) GaN experimental diffraction pattern.

(b) Image contrast is inverted.

(c) Peaks are listed in the peaks table.

(d) Peaks are identified.

(e) The circle are centred on SAED spots.

(f) Binarizing the experimental image can help figure out where the spots are located.

Figure 134: Image processing to identify and list the diffraction spots.
25 Colourise dialogue

The colourise dialogue offers 2 sets of color LookUp Table (Fig. 135). The table contains 56 different LUTs including TemperatureMap and Thermometer-Colors (Figs. 135a, 135b).

25.1 Tool buttons

The tool buttons allow to:

- ![Save](image) : save the selected LUT set as an image.
- ![Clipboard](image) : transfer the dialogue to the clipboard.

![Colourise dialogue](image)

(a) Color LUTs set 1.  
(b) Color LUTs set 2.

Figure 135: Colourise dialogue.
Figure 136: GaN SAED pattern with TemperatureMap LUT.
26  Holography dialogue

The holography dialogue allows to introduce in HRTEM image simulations the effect of a biprism (Fig. 137a).

26.1  Tool buttons

The tool buttons allow to:

- [ ] : transfer the dialogue to the clipboard.
- [ ] : open associated help file.

Figure 137: Holography dialogue allowing to change the biprism and diffraction settings.
Figure 138: ZnTe HRTEM image simulations without and with some arbitrary biprism settings.
27 Electron powder pattern

Figure 139: Table of ZnTe structure factors.

27.1 Tool buttons

The tool buttons allow to:

- : print the table.
- : save the table.
- : transfer the dialogue to the clipboard.
- : display a help file.
28 Rings pattern

Figure 140: Table of ZnTe structure factors.

28.1 Tool buttons

The tool buttons allow to:

- : print the table.
- : save the table.
- : transfer the frame to the clipboard.
- : make a table with different maximum (hkl) indices.
- : reduce the table (Fig. 163).
- : display a powder pattern (Fig. 120).
- : display a ring pattern (Fig. 140).
Figure 141: Table of non-equivalent ZnTe structure factors and their multiplicity.
29  Atomic Form Factor

The Atomic Form Factors (or electron scattering factors) are collected in tables referred by the authors of the tabulation (Fig. ??). The AFF tabulations use different approximations. For simple qualitative calculations the Doyle-Turner/Smith-Burge tabulation is good and pretty equivalent to the others up to element atomic number 40-42. The best tabulations have been provided by Weickenmeier-Kohl since the absorption potential includes the calculation of Thermal Diffuse Scattering within the Einstein approximation (un-correlated atoms vibration).

The source of the AFF’s are provided by the following references:


Accurate AFFs are necessary to compute the Atomic Scattering Amplitude as a function of the reduced scattering angle ($\sin \theta / \lambda$). A detailed comparison as well as a new parametrisation of the electron scattering factors has been provided recently by I. Lobato and D. Van Dyck32. These authors conclude that their new tabulation is an order of magnitude better than the previous ones. This tabulation is not yet introduced in jems.

29.1 Tool buttons

The tool buttons allow to:

- ☞: print the table.
- ☐: save the table.
- ☘: transfer the dialogue to the clipboard.
- ☘: display a help file.

29.2 Popup menu

A **Atomic Scattering Amplitude** (ASA or **Electron Scattering Amplitude**) plot shows the amplitude of the electron scattering as a function of the reduced scattering angle $\frac{\sin \theta}{\lambda}$ (independent of the electron wavelength). The ASA plot is created when any entry of the tables is selected (mouse click).

The popup menu attached to the ASA plots allows to:
- **Print**: print the AFF plot.
- **Save**: save the AFF plot.
- **Compare ASA’s as Notebook**: create a Mathematica notebook that compares the AFF’s of the different sources.
- **Log scale**: plot the AFF using a log scale.
- **Save ASA plot as Notebook**: save the ASA plot as a Mathematica notebook.
- **Save ASA table as Notebook**: save the ASA table as a Mathematica notebook at $\frac{\sin \theta}{\lambda} = 0$ (Fig. 144).
- **Scale x n**: set the ordinate scale of the plot.
- **Transfer to clipboard**: transfer the plot to the clipboard.

Figure 143: Fe atomic form factor (WKc) as a function of $\frac{\sin \theta}{\lambda} = 0$. 

152
(a) Doyle-Turner and Smith-Burge atomic form factors.
(b) Earl J. Kirkland atomic form factors.
(c) Peng-Ren-Dudarev-Whelan atomic form factors.
(d) Weickenmeier-Kohl atomic form factors.
(e) Weickenmeier-Kohl (with core absorption) atomic form factors.
(f) X-Ray (Mott formula) atomic form factors.
(g) A particular AFF source is selected using these radio buttons.

Figure 144: Comparison of the Electron Scattering Amplitudes of the different references at $\frac{\sin \theta}{\lambda} = 0$.

Fig. ?? compares the electron scattering amplitudes from the different references for selected $\frac{\sin \theta}{\lambda}$ values. It shows that the EJK, WK, WKC and XRay plots are pretty similar for all elements and the selected $\frac{\sin \theta}{\lambda}$ values.

Fig. 147 plots the scattering angle $\theta$ as a function of the reciprocal distance $s$ for selected accelerating voltages.
Figure 145: AFF sources.

Figure 146: Comparison of the Electron Scattering Amplitudes of the different references at selected $\frac{\sin \theta}{\lambda}$ values.

(a) $\frac{\sin \theta}{\lambda} = 0 \text{ [nm}^{-1}]$.  
(b) $\frac{\sin \theta}{\lambda} = 1 \text{ [nm}^{-1}]$.  
(c) $\frac{\sin \theta}{\lambda} = 2 \text{ [nm}^{-1}]$.  
(d) $\frac{\sin \theta}{\lambda} = 3 \text{ [nm}^{-1}]$.  
(e) $\frac{\sin \theta}{\lambda} = 4 \text{ [nm}^{-1}]$.  
(f) $\frac{\sin \theta}{\lambda} = 5 \text{ [nm}^{-1}]$.  
(g) $\frac{\sin \theta}{\lambda} = 10 \text{ [nm}^{-1}]$.  
(h) $\frac{\sin \theta}{\lambda} = 20 \text{ [nm}^{-1}]$.  
(i) $\frac{\sin \theta}{\lambda} = 50 \text{ [nm}^{-1}]$.  

$\text{DTSB} \blacklozenge, \text{EJK} \blacklozenge, \text{PRDW} \blacklozenge, \text{WK} \blacklozenge, \text{WKc} \blacklozenge, \text{XRay} \blacklozenge$
Figure 147: Scattering angle [mRad] as a function of $s \, [nm^{-1}]$ for selected accelerating voltages [kV]. Note the factor 2 for the conversion $nm^{-1}$ to mRad.
## 30 Structure factors dialogue

![Table of ZnTe structure factors](image)

**Figure 148:** Table of ZnTe structure factors.

### 30.1 Tool buttons

The tool buttons allow to:

- ![Print](image): print the table.
- ![Save](image): save the table.
- ![Clipboard](image): transfer the dialogue to the clipboard.
- ![Maximum](image): make a table with different maximum (hkl) indices.
- ![Reduce](image): reduce the table (Fig. 163).
- ![Electron](image): open electron powder pattern frame (Fig. 139).
- ![Rings](image): open rings pattern frame (Fig. 140).
- ![Help](image): display a help file.
Figure 149: Table of non-equivalent ZnTe structure factors and their multiplicity.
31 Miscellany menu

The Miscellany menu offers possibilities to load .ems images or super-cells (.xyz, .cel formats) and to generate various models of crystal structures.

31.1 Miscellany menu items

The menu items allow to:

- **Load image**: load .ems images (Fig. 150).
- **Load super-cell**: load model structure in .xyz or .cel formats (Fig. 151).
- **Make void**: create a void in a structure (Fig. 152).
- **To core-shell**: create core-shell particles (Fig. 153).
- **To particle**: create spherical or faceted particles (Fig. 155).
- **To precipitate**: create a precipitate in a matrix (Fig. 156).
- **To slices**: slice a crystal structure (Fig. 158).
- **To triclinic**: duplicate and rotate a crystal structure (Fig. 160).
31.1.1 Load image

Figure 150: Miscellany menu Load image frame.
31.1.2 Load super-cell

Figure 151: Miscellany menu **Load super-cell** frame.
31.1.3 Make void

Figure 152: Miscellany menu **Make void** frame.
31.1.4 To core-shell

Frame (Fig. 153) allows to create core-shell (spherical) particles. Regular .txt crystal structures are loaded for the core (here Au, duplicated \( n_x \times n_y \times n_z \) times and the shell (here \( SiO_2 \) duplicated \( n'_x \times n'_y \times n'_z \) times). The particle is placed in a box and the model can be sliced into thinner sub-slices ready for multislice calculations.

Figure 153: Miscellany menu To core-shell frame.
Figure 154: To core-shell 3D-views. The model is embedded in a box of dimensions large enough to avoid "wrap around" artefacts during the multislice image calculation.
### 31.1.5 To particle

![Figure 155: Miscellany menu To particle frame.](image)
31.1.6 To precipitate

Figure 156: Miscellany menu To precipitate frame.
Figure 157: To precipitate 3D-views. The model is embedded in a box of dimensions large enough to avoid "wrap around" artefacts during the multislice image calculation.
31.1.7 To slices

Figure 158: Miscellany menu **To slices** frame.

(a) Table of slices.  
(b) 3D-view of a slice.

Figure 159: Table of slices and 3D-view of a single slice or the stack of slices.
31.1.8 To triclinic

Figure 160: Miscellany menu To triclinic frame.

(a) To triclinic model 3D-view.  
(b) Duplicated void model 2x2x1

Figure 161: To triclinic simple model and duplicated void model 3D-view.
32 Thickness

![Figure 162: Thickness measurement.](image)

### 32.1 Tool buttons

The tool buttons allow to:

- 🖨️: print the table.
- 📄: save the table.
- 📚: transfer the frame to the clipboard.
- 📊: load a CBED image.
- 🌪️: move the Center of the Laue Circle (CLC) down.
- 📊: move the CLC up.
- 📚: move the CLC left.
- 📚: move the CLC right.
- 📊: make a table with different maximum (hkl) indices.
- 📊: reduce the table (Fig. 163).
• ▶ : display a powder pattern (Fig. 120).
• ⊙ : display a ring pattern (Fig. 140).
• 📚 : display a help file.

Figure 163: Table of non-equivalent ZnTe structure factors and their multiplicity.
Figure 164: ZnTe perspective view.
33.1 Popup menu

The popup menu (Fig. 165) associated with the view allows to transfer the view to the clipboard as well as to save, print, create a Mathematica notebook or generate a powder pattern. It controls also the creation of the movies.

33.2 Tool buttons

The tool buttons allow to:

- : print the table.
- : save the table.
- : transfer the frame to the clipboard.
- : open the Specimen dialogue (Fig. 88a).
- : display a Powder pattern (Fig. 120).
- : duplicate the unit cell $n_x \times n_y \times n_z$ (Fig. 166b).
- : display a help file.

Figure 165: 3-D view popup menu.
33.3 Tabs

3-D view controls are collected in the following tabs in order to define:

- **Atoms**: the atoms colour and size as well as bonding and resolution (Fig. 167a).
- **Direction**: the viewing direction (Fig. 167b).
- **Display**: the 3-D perspective details (Fig. 167c).
- **Duplicate**: the model duplication (Fig. 167d).
- **View**: the view type (Fig. 167e).
The **Atoms** and **Display** tabs are organized in sub-tabs that control the colour and size of the atoms as well as the bonding and resolution of the views (Figs. 168a, 168b, 168c, 168d, 168e, 168f, 168g, 168h). They allow, for example, to create **Black & White** figure (169a) or to look at (hkl) planes (Fig. 169b).
(a) Zn colour and size.
(b) Te colour and size.
(c) Define the bonding of ZnTe.
(d) Resolution of the spheres and bonds.
(e) 3D-view details.
(f) Cut thickness and distance to middle of model (when Cut check-box is selected).
(g) Movie controls.
(h) Cut plane selection (when Cut check-box is selected).

Figure 168: Atoms and Display Tabs.
Figure 169: Modified 3-D views.
34 Indexing SAED patterns

Figure 170: Indexing SAED patterns.

34.1 Tool buttons

The tool buttons allow to:

- : print the image.
- : save the image.
- : transfer the frame to the clipboard.
- : open an image.
- : process image.
- : start indexing process.
- : show diffractogram (when an HRTEM image has been loaded).
- : magnify part of image.
- : tabulate the image.
• 📜: open keeper dialogue (Fig. 94).
• 📖: display a help file.
34.2 Tabs

(a) Rotation of the spot indexing mask.

(b) Table of the crystal files selected for the indexing.

(c) Mask showing the spots selected for indexing.

(d) Controls of the microscope parameters.

Figure 171: Controls and tabs of SAED patterns indexing.
(a) Options to control the indexing process, in particular the number of spots used by the indexing.

(b) Image processing tab.

(c) Controls to set the scale of the experimental SAED pattern or diffractogram.

(d) Controls to define the spot distances and angles.

Figure 172: Controls and tabs of SAED patterns indexing.
34.3 Example

The image processing tab is available in several jems frame. It can be used to automatically identify the center of spots on diffraction patterns (Fig. 173).

(a) GaN experimental diffraction pattern.  
(b) Image contrast is inverted.

(c) Peaks are listed in the peaks table.  
(d) Peaks are identified.

(e) The circle are centred on SAED spots ( ).  
(f) Binarizing the experimental image can help figure out where the spots are located.

Figure 173: Indexing SAED to identify and list the diffraction spots.
The ADF imager frame is shown on Fig. 174. It allows to calculate Bright-Field, Dark Field, HAADF as well as Sector Detector images. The ADF imager moves a probe on a projected structure and integrate the scattered signal on an annular detector that is controlled using the BF/ADF detector dialogue (Fig. 175). When large super-cells are imaged it is very useful to define the parent unit cell crystal and imaging zone axis (Fig. 176c) since the diffraction pattern of the detector dialogue will be created using the unit cell.

The ADF simulation computes 4 Bright and Dark images at once. The size of the first bright or dark field detector is selected (Fig. 175) and the size of the three supplementary ones is increased by 5, 10, 15, 20 or 25 milliradians.
Figure 175: The ADF detector dialogue allows to set the size and position of the Bright and Dark field detectors as well as the Sector detector.

35.1 Tool buttons

The tool buttons of the HRTEM imager allow to:

- ☞: print the selected ADF image tab.
- ☞: save the selected ADF image tab.
- ☞: transfer the ADF frame to the clipboard.
- ☞: display the interpolated ADF image and allows tabulating the selected ADF image.
- ☞: open the Microscope dialogue (Fig. 112).
- ☞: open the ADF detector dialogue (Fig. 175).
- ☞: open the Specimen dialogue (Fig. 88a).
- ☞: open the Transfer function frame (Fig. 101).
- ☞: open the image contrast controls.
• 📝: open the associated help dialogue.

35.2 Tabs

The imaging controls are organised in several tabs aimed at:

• **Iteration**: defining the super-cells stack (Fig 176a).
• **Multislice**: (Fig 176b)
• **Options**: (Fig 176c).
• **Sampling**: (Fig 176d).
• **Scanning**: (Fig 176e).
• **Signal**: (Fig 176f).
(a) Stack of super-cells and total specimen thickness.

(b) Controls the potential generation method (Analytic recommended), the multislice sampling and approximation, the optical potential calculation (not necessary when WK or WKc AFF are selected) and the Frozen lattice approximation and configurations number.

(c) Selects Atomic Form Factors source, allows Bright, Dark, Sector or HAADF image calculation and when checkbox Save is selected saves all the calculated images.

(d) Displays information about the detectors sizes and the maximum scattering angle of the multislice calculation.
Figure 177: **Bright field, Dark field, Sector** and **HAADF** image tabs.
Figure 178: Projection, Projected potential, absorption potential, Fresnel propagator image tabs.
Figure 179: Phase object, Power spectrum, Bright field detector, Dark field detector image tabs.
Figure 180: Dark field detector and Wave-function image tabs.
(a) Probe dialogue with probe shown on projected potential image.

(b)

(c)

Figure 181: **Probe** dialogue and **Aberrated probe** shape 2-D and 3-D (3-fold astigmatism).

The wave-front aberration $W_{ij}$ defines the $i^{th}$ power of the radial angle and the
$j^{fold}$ azimuthal angle $^{33}$.

$^{33}$The chromatic aberration is $W_{00}$. 
36 Probe imager

The **Probe imager** dialogue sets the probe position and properties (shape) before starting any ADF image calculation (Fig. 182). Depending on the size of the scanned area with respect to the size of the ADF calculation, the probe position will be placed at the middle of the projected potential image or at the middle of the scanned area (Fig. 185a). When smaller than the calculation size the position of the scan area is selectable using the pointer. The probe shape (Fig. 185b) is displayed and its shape changes according to the aberrations, coherence or microscope settings.

![Figure 182: Probe imager dialogue.](image)

Closing the dialogue will start the ADF image calculation.

36.1 Tool buttons

The tool buttons allow to:

- **Reset** button resets the aberrations and other settings to their default value
• ⌨: print either the probe position or probe shape image.
• 📝: save the probe position or probe shape image.
• 🖼: transfer the frame to the clipboard.
• 🎨: open the Keeper dialogue.
• 📚: display a help file.

### 36.2 Tabs

The probe shape and position depends on the aberrations, coherence and several microscope settings that are collected in the following tabs:

- **Aberrations**: to set the aberrations from order 0 (chromatic aberration) to 8 (Fig. 183a)\(^{35}\).
- **Coherence**: to set the coherence of the illumination (Fig. 184a).
- **Drift&Noise**: to set the TMagnetic noise and vibration (Fig. 184c).
- **Microscope**: to set the aperture diameter, accelerating voltage and virtual source size (Fig. 184d).

![Figure 183: Probe aberrations.](image)

---

\(^{35}\)The formula of a particular aberration (in orthogonal axes) is displayed when its value is modified either using the table or the sliders.
(a) Coherence settings of the microscope illumination.

(b) Contrast tab to modify the contrast of the probe image.

(c) Thermal Magnetic noise and vibration settings.

(d) Probe defocus is set using the $W_{20}$ control (Fig. 183a).

Figure 184: Coherence, Contrast, Drift&Noise, Microscope settings.

The probe position image offers a popup menu that allows to save, print and transfer the image to the clipboard. The popup attached to the probe image allows to create a stack of defocused probe images (Fig. 186a) showing the probe shape either along the $O_z$ axis or laterally along the $O_x$ or $O_y$ axes and to display the probe profile and labelled circles (Fig. 186b).
(a) The probe position is placed at the center of the scanned area (controlled by pointer).

(b) Probe shape is defined using the controls collected in the left tabs.

Figure 185: Probe position and probe shape.
(a) Lateral view of the probe shape as a function of defocus, defocus step 0.1 nm and optimum defocus (-0.03 nm) at the middle of the 512 images stack.

Figure 186: Lateral probe view and probe profile (obtained using the attached popup menu).

(b) Probe profile and labelled circles.